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FILE LAST UPDATED: 21 Apr 2008 (20080421/ED)

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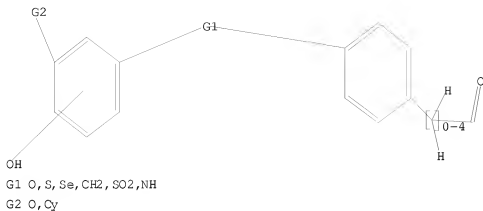
<http://www.cas.org/infopolicy.html>

=>
Uploading C:\Program Files\Stnexp\Queries\6100b.str

L1 STRUCTURE UPLOADED

=>
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L1 HAS NO ANSWERS
L1 STR

10/923,271



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:57:01 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1421473 TO ITERATE

70.3% PROCESSED 1000000 ITERATIONS

164 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.11

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1421473 TO 1421473

PROJECTED ANSWERS: 188 TO 278

L2 164 SEA SSS FUL L1

L3 41 L2

=> s l3 and py<2003

22929827 PY<2003

L4 21 L3 AND PY<2003

=> d 1-21 ibib abs hitstr

L4 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:675334 CAPLUS

DOCUMENT NUMBER: 138:4461

TITLE: Synthesis of 3-(3,4-dihydroxyphenyl)-propionic acid derivatives by N-coupling of amines using laccase

AUTHOR(S): Mikolasch, Annett; Hammer, Elke; Jonas, Ulrike; Popowski, Katrin; Stielow, Anne; Schauer, Frieder

CORPORATE SOURCE: Institut für Mikrobiologie, Ernst-Moritz-Arndt-Universität Greifswald, Greifswald, D-17489, Germany

SOURCE: Tetrahedron (2002), 58(38), 7589-7593
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

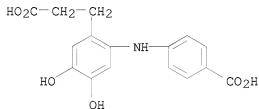
OTHER SOURCE(S): CASREACT 138:4461

AB Derivatization of the natural compound 3-(3,4-dihydroxyphenyl)-propionic acid (dihydrocaffeic acid) can be achieved by laccase-catalyzed N-coupling of aromatic and aliphatic amines. Incubation of 3-(3,4-dihydroxyphenyl)-propionic acid and 4-aminobenzoic acid with laccase in aqueous medium and in the presence of oxygen yielded 3-[6-(4-carboxyphenyl)amino]-3,4-dihydroxyphenyl-propionic acid as the main product (>80%). Reaction with hexylamine resulted in 3-(6-hexylamino-3,4-dihydroxyphenyl)-propionic acid as the only product (60%).

IT 476614-58-1P
RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(laccase-catalyzed N-coupling of aromatic and aliphatic amines in preparation of 3-(3,4-dihydroxyphenyl)-propionic acid derivs.)

RN 476614-58-1 CAPLUS

CN Benzenepropanoic acid, 2-[(4-carboxyphenyl)amino]-4,5-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:633267 CAPLUS

DOCUMENT NUMBER: 137:325735

TITLE: Synthesis and characterization of hyperbranched polybenzoxazoles

AUTHOR(S): Hong, Chi-Sun; Jikei, Mitsutoshi; Kakimoto, Masa-Aki

CORPORATE SOURCE: Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, 152-8550, Japan

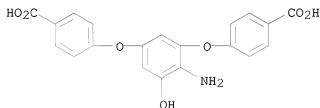
SOURCE: Journal of Photopolymer Science and Technology (2002), 15(2), 219-222
CODEN: JSTEEW; ISSN: 0914-9244

PUBLISHER: Technical Association of Photopolymers, Japan

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Polymerization of 3,5-bis(4-carboxyphenoxy)-2-aminophenol hydrochloride in NMP
 in the presence of Et₃N, di-Ph (2,3-dihydro-2-thioxo-3-benzoxazolyl)phosphonate, and 2-amino-4-tert-butylphenol end-capping agent gave a soluble poly(o-hydroxyamide) which was cyclized by heat or by reaction in polyphosphoric acid at 130° for 6 h to the corresponding polybenzoxazole which exhibited good solubility in aprotic solvents and thermal stability.

IT 473702-29-3P, 3,5-Bis(4-carboxyphenoxy)-2-aminophenol
 hydrochloride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (monomer; synthesis and characterization of heat-resistant hyperbranched polybenzoxazoles from bis(carboxyphenoxy)aminophenol hydrochloride)

RN 473702-29-3 CAPLUS
 CN Benzoic acid, 4,4'-[(4-amino-5-hydroxy-1,3-phenylene)bis(oxy)]bis-, hydrochloride (9CI) (CA INDEX NAME)



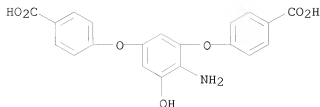
● HC1

IT 473702-30-6DP, 3,5-Bis(4-carboxyphenoxy)-2-aminophenol
 hydrochloride homopolymer, reaction products with amino-tert-butylphenol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (polybenzoxazole precursor; synthesis and characterization of heat-resistant hyperbranched polybenzoxazoles from bis(carboxyphenoxy)aminophenol hydrochloride)

RN 473702-30-6 CAPLUS
 CN Benzoic acid, 4,4'-[(4-amino-5-hydroxy-1,3-phenylene)bis(oxy)]bis-, hydrochloride, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 473702-29-3
 CMF C20 H15 N O7 . C1 H

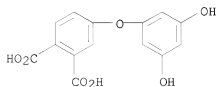


● HCl

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:207561 CAPLUS
 DOCUMENT NUMBER: 136:248400
 TITLE: Soluble multibranched polyimides and manufacturing methods therefor
 INVENTOR(S): Kakimoto, Masaaki; Terazakai, Mitsutoshi; Yamanaka, Kazuhiro
 PATENT ASSIGNEE(S): Rikogaku Shinkokai, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

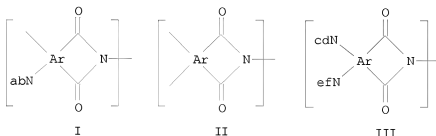
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002080597	A	20020319	JP 2000-269155	20000905 <--
PRIORITY APPLN. INFO.:			JP 2000-269155	20000905
AB	Polyimides are prepared from (R1HN)(R2HN)Ar(CO2R3)(CO2R4), where Ar is a tetravalent organic groups, R1, R2 = H or Me3Si, R1 = R2 or R1 ≠ R2, R3, R4 = C1-10 alkyl, aryl, or Me3Si, R3 = R4 or R3 ≠ R4. Thus, 3,5-bis(4-aminophenoxy)diphenyl ether 3',4-dicarboxylic acid mono-Me ester was prepared and polymerized			
IT	332837-59-9P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (manufacture of aromatic diamine dicarboxylic acid esters for soluble multibranched polyimides)			
RN	332837-59-9 CAPLUS			
CN	1,2-Benzenedicarboxylic acid, 4-(3,5-dihydroxyphenoxy)- (CA INDEX NAME)			



L4 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:252965 CAPLUS
 DOCUMENT NUMBER: 134:281290
 TITLE: Polyimides with good solubility and their manufacture
 INVENTOR(S): Kakimoto, Masaaki; Terazakai, Mitsutoshi; Yamanaka, Kazuhiro
 PATENT ASSIGNEE(S): Zaidan Hojin Rikogaku Shinkokai, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 40 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001098071	A	20010410	JP 2000-200862	20000703 <--
JP 3546303	B2	20040728		

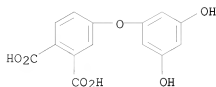
PRIORITY APPLN. INFO.: JP 1999-210653 A 19990726
 GI



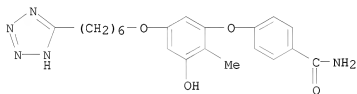
AB The polyimides, useful for elec. insulators, etc., comprising repeating units of I, II, and III (Ar = tetravalent organic group; abN, cdN, efN = unsubstituted amino, cyclic amide, C1-10-alkyl, aryl, trimethylsilyl, C2-7-hydrocarbylene, mono- or divalent acyl-substituted amino; cdN and efN may form NHXNH; X = hydrocarbylene, acyl) are manufactured Thus, 4-[3,5-bis(4-aminophenoxy)phenoxy]-1,2-benzenedicarboxylic acid monomethyl ester was polymerized, treated with heptanoyl chloride, and heated in the presence of acetic anhydride to give a polyimide with good solubility in organic solvents.

IT 332837-59-9P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (manufacture of polyimides with good solubility)

RN 332837-59-9 CAPLUS
 CN 1,2-Benzenedicarboxylic acid, 4-(3,5-dihydroxyphenoxy)- (CA INDEX NAME)



L4 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:231090 CAPLUS
 DOCUMENT NUMBER: 135:40429
 TITLE: Computer-aided design of molecules possessing
 antiasthmatic properties based on computer QSAR
 analysis
 AUTHOR(S): Shilova, E. V.
 CORPORATE SOURCE: All-Russia Scientific Center for Safety Testing of
 Biologically Active Substances, Ministry of Public
 Health of Russian Federation, Kupavna, Russia
 SOURCE: Pharmaceutical Chemistry Journal (Translation of
 Khimiko-Farmatsevticheskii Zhurnal) (2000),
 34(8), 419-423
 CODEN: PCJOAU; ISSN: 0091-150X
 PUBLISHER: Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The purpose of this study was to establish pharmacophores and
 antipharomacophores for the antiasthmatic properties and to design mols.
 capable of acting simultaneously by several mechanisms.
 IT 345218-05-5
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
 (Uses)
 (computer-aided design of mols. possessing antiasthmatic properties
 based on computer QSAR anal.)
 RN 345218-05-5 CAPLUS
 CN Benzamide, 4-[3-hydroxy-2-methyl-5-[[6-(1H-tetrazol-5-
 yl)hexyl]oxy]phenoxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:490074 CAPLUS
 DOCUMENT NUMBER: 133:248854
 TITLE: Novel tert-Butyl Migration in Copper-Mediated Phenol

Ortho-Oxygenation Implicates a Mechanism Involving Conversion of a 6-Hydroperoxy-2,4-cyclohexadienone Directly to an o-Quinone

AUTHOR(S): Mandal, Subrata; Macikenas, Dainius; Protasiewicz, John D.; Sayre, Lawrence M.

CORPORATE SOURCE: Department of Chemistry, Case Western Reserve University, Cleveland, OH, 44106-7078, USA

SOURCE: Journal of Organic Chemistry (2000), 65(16), 4804-4809

PUBLISHER: CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: American Chemical Society

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:248854

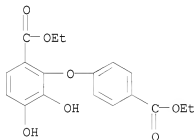
AB Copper mediated ortho-oxygenation of phenolates may proceed through the generation of a 6-peroxy-2,4-cyclohexadienone intermediate. To test this theory, we studied the fate of sodium 4-carbethoxy-2,6-di-tert-butylphenolate, where the ortho-oxygenation sites are blocked by tert-Bu groups. Using the Cu(I) complex of N,N-bis(2-(N-methylbenzimidazol-2-yl)ethyl)benzylamine, isolation of the major oxygenated product and characterization by single-crystal X-ray crystallog. and NMR spectroscopy revealed it to be 4-carbethoxy-3,6-di-tert-butyl-1,2-benzoquinone, resulting from a 1,2-migration of a tert-Bu group. The independently prepared 6-hydroperoxide is transformed by the Cu(I)- (or Cu(II)-) ligand complex to the same o-quinone. The observed 1,2-migration of the tert-Bu group appears to reflect an electron demand created by rearrangement of the postulated peroxy intermediate. A mechanism proceeding alternatively through a catechol and subsequent oxidation to the o-quinone seems ruled out by a control study demonstrating that the requisite intermediate to catechol formation would instead eliminate the 2-tert-Bu group.

IT 296252-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(novel tert-Bu migration in copper-mediated phenol ortho-oxygenation implicates a mechanism involving conversion of a 6-hydroperoxy-2,4-cyclohexadienone directly to an o-quinone)

RN 296252-78-3 CAPLUS

CN Benzoic acid, 2-[4-(ethoxycarbonyl)phenoxy]-3,4-dihydroxy-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

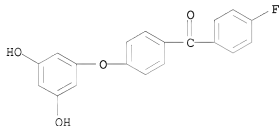
L4 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2000:216941 CAPLUS
 DOCUMENT NUMBER: 132:322237
 TITLE: Preparation of poly[(ether)-(ether ether ketone)]
 dendrimers by the convergent method
 AUTHOR(S): Morikawa, Atsushi; Ono, Katsumichi
 CORPORATE SOURCE: Department of Materials Science, Faculty of
 Engineering, Ibaraki University, Hitachi, 316-8511,
 Japan
 SOURCE: Polymer Journal (Tokyo) (2000), 32(3),
 255-262
 CODEN: POLJB8; ISSN: 0032-3896
 PUBLISHER: Society of Polymer Science, Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB New highly branched poly[(ether)-(ether ether ketone)] dendrimers were synthesized by the convergent approach using two building blocks, 3,5-dihydroxybenzyl alc., (I), and 3,5-dihydroxy-4'-(4-fluorobenzoyl)diphenyl ether, (II), alternatively. The reaction of p-fluorobenzonitrile and I gave 3,5-bis(4-cyanophenoxy)benzyl alc. (the first generation dendron, G1-OH). After G1-OH was converted to 3,5-bis(4-cyanophenoxy)benzyl bromide (G1-Br), the resultant benzylic bromide functionality was allowed to react with II to yield the second-generation dendron (G2-F). The third-generation dendron (G3-OH) was obtained by the reaction of G2-F and I, and the fourth-generation dendron (G4-F) was obtained by reaction of G3-Br derived from G3-OH, with II. Finally, dendrimers, Den-(G2)3 and Den-(G4)3 were synthesized by reaction of G2-F and G4-F with trifunctional core, resp. Anal. was made of these structurally unambiguous dendrons and dendrimers by gel permeation chromatog. (GPC) and matrix-assisted laser desorption ionization time of flight (MALDI-TOF) mass spectroscopy. ¹H and ¹³C NMR spectra were consistent with the structures of these dendrons and dendrimers.

IT 266370-71-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of poly[(ether)-(ether ether ketone)] dendrimers by convergent method)

RN 266370-71-2 CAPLUS
 CN Methanone, [4-{3,5-dihydroxyphenoxy}phenyl](4-fluorophenyl)- (CA INDEX NAME)

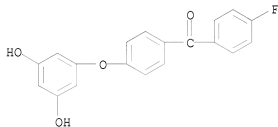


IT 266370-75-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of poly[(ether)-(ether ether ketone)] dendrimers by convergent

method)
 RN 266370-75-6 CAPLUS
 CN Methanone, [4-(3,5-dihydroxyphenoxy)phenyl] (4-fluorophenyl)-, polymer with
 5-(hydroxymethyl)-1,3-benzenediol (9CI) (CA INDEX NAME)

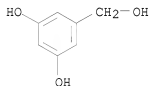
CM 1

CRN 266370-71-2
 CMF C19 H13 F O4



CM 2

CRN 29654-55-5
 CMF C7 H8 O3



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:216938 CAPLUS
 DOCUMENT NUMBER: 132:334958
 TITLE: Preparation of poly(ether ether ketone) dendrimers by
 the divergent method
 AUTHOR(S): Morikawa, Atsushi; Ono, Katsumichi
 CORPORATE SOURCE: Department of Materials Science, Faculty of
 Engineering, Ibaraki University, Hitachi, 316-8511,
 Japan
 SOURCE: Polymer Journal (Tokyo) (2000), 32(3),
 234-242
 CODEN: POLJB8; ISSN: 0032-3896
 PUBLISHER: Society of Polymer Science, Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB New highly branched poly(ether ether ketone) dendrimers were synthesized

by the divergent approach through aromatic nucleophilic substitution reactions. 3,5-Dimethoxy-4'-(4-fluorobenzoyl)diphenyl ether, 1, and 1,3,5-tris[p-(3,5-dihydroxyphenoxy)phenyl]benzene, G0-OH, were used as a building block and starting core, resp. The reaction of 1 with G0-OH gave the first-generation dendrimer (G1-OMe), which possessed 12 methoxy groups on the periphery. After the methoxy groups were converted to hydroxy groups by treatment with pyridine hydrochloride, the resultant phenol functionality (G1-OH) was allowed to react with 1 to yield the second-generation dendrimer (G2-OMe) which possessed 24 methoxy groups. By repeating these procedures G3-OMe dendrimer and G3-OH dendrimer possessing 48 methoxy and hydroxy groups, resp., on the periphery were obtained. ¹H and ¹³C NMR spectra were consistent with the structures of these dendrimers. Mol. wts. and mol. weight distribution determined by gel permeation chromatog. indicated that the dendrimers possessed remarkably narrow mol. weight distribution. Anal. was made of these structurally unambiguous dendrimers by matrix-assisted laser desorption ionization time of flight (MALDI-TOF) mass spectroscopy. The characteristics of these dendrimers, Gn-OMe and Gn-OH, such as solubility and thermal properties were compared.

IT 267421-53-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(dendritic; preparation of poly(ether ether ketone) dendrimers by divergent method)

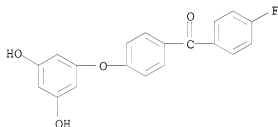
RN 267421-53-4 CAPLUS

CN Methanone, [4-(3,5-dihydroxyphenoxy)phenyl](4-fluorophenyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 266370-71-2

CMF C19 H13 F O4



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:513659 CAPLUS

DOCUMENT NUMBER: 131:257279

TITLE: Synthesis of fluorinated polyphenyl ethers by reaction of polyfluorinated cyclohexadienones with substituted phenols

AUTHOR(S): Kovtonyuk, V. N.; Kobrina, L. S.

CORPORATE SOURCE: Novosibirsk Institute of Organic Chemistry, Siberian

Division, Russian Academy of Sciences, Novosibirsk, 630090, Russia

SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1999), 35(1), 74-79
CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

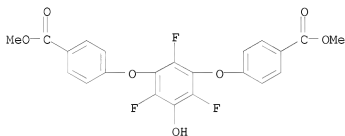
LANGUAGE: English

AB Perfluoro(4-phenoxy-2,5-cyclohexadienone) reacts with sodium 4-nitro- and 4-methoxycarbonylphenoxides in glyme at 65°C to give the corresponding 2,4,6-trifluoro-3,5-bis(aryloxy)-4-[2,4,6-trifluoro-3,5-bis(aryloxy)phenoxy]-2,5-cyclohexadienones. Reduction of the latter to phenols, followed by reaction with perfluorotoluene, results in formation of branched polyfluorinated polyphenyl ethers containing NO₂ and CO₂CH₃ functional groups. Reduction of the dinitro polyphenyl ether yields the corresponding diamino derivative. A similar reaction sequence gives rise to a linear polyphenyl ether, starting from 6-chloro-2,3,4,5,6-pentafluoro-2,4-cyclohexadien-1-one and tetrafluoroethanol.

IT 245126-30-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorinated polyphenyl ethers by reaction of polyfluorinated cyclohexadienones with phenols)

RN 245126-30-1 CAPLUS

CN Benzoic acid, 4,4'-[(2,4,6-trifluoro-5-hydroxy-1,3-phenylene)bis(oxy)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:348617 CAPLUS

DOCUMENT NUMBER: 131:155777

TITLE: Phenolics and flavonoids from Haematoxylon campechianum

AUTHOR(S): Kandil, F. E.; Michael, H. N.; Ishak, M. S.; Mabry, T. J.

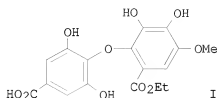
CORPORATE SOURCE: Chemistry of Tanning Materials and Proteins Department, National Research Centre, Cairo, Egypt

SOURCE: Phytochemistry (1999), 51(1), 133-134
CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English
GI

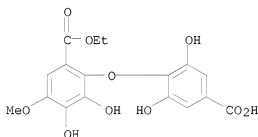


AB One new natural phenolic, the 5'-O-methyl-7'-Et ester I of p-dehydridigallic acid, was isolated and identified from the bark of Haematoxylon campechianum. In addition, two known flavonoids, quercetin 3-O-Me ether and genistein and three known phenolics, gallic acid, Me gallate and Et gallate, were also isolated.

IT 237067-27-5P
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and structure of phenolics and flavonoids from Haematoxylon campechianum)

RN 237067-27-5 CAPLUS

CN Benzoic acid, 2-(4-carboxy-2,6-dihydroxyphenoxy)-3,4-dihydroxy-5-methoxy-, 1-ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:297219 CAPLUS

DOCUMENT NUMBER: 127:17460

TITLE: A convenient synthesis of 2-alkylated 1,4-benzenediols

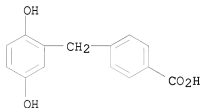
AUTHOR(S): Ozaki, Yutaka; Hosoya, Ayako; Okamura, Kyoko; Kim, Sang Won

CORPORATE SOURCE: Faculty Pharmaceutical Sciences, Josai University, Sakado, 350, Japan

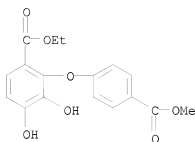
SOURCE: Synlett (1997), (4), 365-366

PUBLISHER: CODEN: SYNLES; ISSN: 0936-5214
Thieme

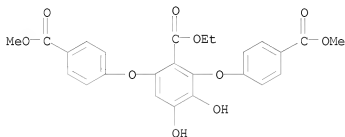
DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 127:17460
 AB Reaction of 1,4-cyclohexanedione with a variety of aldehydes in the presence of metal halides generated the 2-alkylated 1,4-benzenediols in good yields without any aromatic byproducts.
 IT 190597-10-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of alkylbenzenediols from cyclohexanedione and aldehydes)
 RN 190597-10-5 CAPLUS
 CN Benzoic acid, 4-[(2,5-dihydroxyphenyl)methyl]- (CA INDEX NAME)



L4 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1996:680694 CAPLUS
 DOCUMENT NUMBER: 126:103762
 TITLE: Copper-catalyzed ortho-oxidation of phenols by dioxygen (tyrosinase mimics) do yields catechols as primary products
 AUTHOR(S): Maumy, M.; Capdevielle, P.
 CORPORATE SOURCE: Laboratoire de Chimie Organique de l'ESPCI, associe au CNRS, 10 rue Vauquelin, Paris, 75231/05, Fr.
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 159-166
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 126:103762
 AB Evidences are provided that catechols [as copper(II)catecholates] are the actual primary products of copper-mediated (catalyzed) ortho-selective oxidation of phenols, on the contrary to a recent claim reporting direct generation of ortho-quinones.
 IT 186041-68-9P 186041-70-3P
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (catechols as primary products from copper-catalyzed ortho-oxidation of phenols by dioxygen (tyrosinase mimics))
 RN 186041-68-9 CAPLUS
 CN Benzoic acid, 3,4-dihydroxy-2-[4-(methoxycarbonyl)phenoxy]-, ethyl ester (CA INDEX NAME)



RN 186041-70-3 CAPLUS
 CN Benzoic acid, 3,4-dihydroxy-2,6-bis[4-(methoxycarbonyl)phenoxy]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:537861 CAPLUS

DOCUMENT NUMBER: 125:275352

TITLE: Galloyl-Derived Orthoquinones as Reactive Partners in Nucleophilic Additions and Diels-Alder Dimerizations: A Novel Route to the Dehydrodigalloyl Linker Unit of Agrimoniin-Type Ellagitannins

AUTHOR(S): Feldman, Ken S.; Quideau, Stephane; Appel, Heidi M.

CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Journal of Organic Chemistry (1996), 61(19), 6656-6665

CODEN: JOCEAH; ISSN: 0022-3263

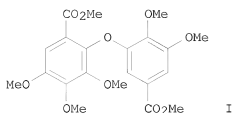
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:275352

GI



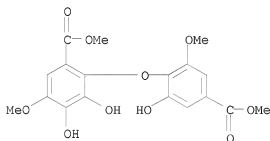
AB Orthochloranil-mediated oxidation of galloyl mono ethers furnishes the derived orthoquinones in excellent yield. These reactive electrophiles participate in a variety of nucleophilic addition reactions with heteroat. and carbanionic partners. In addition, Lewis acid-mediated dimerization of the orthoquinones provides an efficient route to dehydrodigalloyl-type diaryl ether units, e.g. I, characteristic of several ellagitannin natural products. The implications for ellagitannin biosynthesis and gallotannin-protein covalent attachment are discussed.

IT 182183-02-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(galloyl-derived orthoquinones as reactive partners in nucleophilic addns. and Diels Alder dimerizations in preparation of dehydrodigalloyl linker unit of agrimoniin-type ellagitannins)

RN 182183-02-4 CAPLUS

CN Benzoic acid, 3,4-dihydroxy-2-[2-hydroxy-6-methoxy-4-(methoxycarbonyl)phenoxy]-5-methoxy-, methyl ester (CA INDEX NAME)



L4 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:52555 CAPLUS

DOCUMENT NUMBER: 50:52555

ORIGINAL REFERENCE NO.: 50:10051g-i,10052a-c
TITLE: Synthesis of 3,4-diethoxydiphenyl ether-4',6-dicarboxylic acid

AUTHOR(S): Tomita, Masao; Kugo, Takehiko

CORPORATE SOURCE: Univ. Kyoto

SOURCE: Yakugaku Zasshi (1955), 75, 1350-4

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 4-[6,3,4-HO2C(MeO)2C6H2O]C6H4CO2H (I) (0.5 g.) and 5 ml. AcOH saturated with

HBr at 0° in a sealed tube heated 1 hr. at 105°, cooled, the product washed with water, concentrated in vacuo and the residue extracted with Et2O

gave 0.25 g. 3,4-di-OH analog (II) of I, columns, m. 196-8°.

Methylation of 0.4 g. II in MeOH with CH2N2 in Et2O, removing of the solvent, extracting with Et2O, washing with 3% KOH and saponifying with alc.

KOH

gave I, needles, m. 146-7°. 3,4,6-Me(HO)2C6H2Br (III) (4 g.), m. 92°, in 12 ml. EtOH treated with 1.6 g. NaOH as a 50% aqueous solution and 15 g. Me2SO4 with 6 g. NaOH in 3 portions while heating on a water bath and keeping the reaction alkaline throughout, and the oily layer extracted with Et2O, washed with 10% NaOH, and distilled gave 4.2 g. di-Et ether (IV), b_p 140-50°, plates, m. 62-5°. IV (0.5 g.) in 25 ml. azeotropic mixture of C5H5N-H2O treated portionwise with 1.5 g. KMnO4, heated 2 hrs. on a water bath, the product filtered off, the filtrate concentrated in vacuo, and the residue in water acidified with HCl and recrystd. from MeOH gave 6,3,4-Br(EtO)2C6H2CO2H (V), granules, m. 160-2°. Methylation of 11 g. 3,4-(EtO)2C6H3CO2H by boiling 4 hrs. with 100 ml. MeOH and 10 ml. concentrated H2SO4 gave 12 g. 3,4-(EtO)2C6H3CO2Me (VI), columns, m. 53-4°. VI (11 g.) in 30 ml. AcOH and 9 g. Br in 15 ml. AcOH treated 5 hrs. at 14°, let stand overnight, the product poured into water, extracted with Et2O, washed with 2% NaOH, the Et2O removed and the residue recrystd. from MeOH gave 10 g. 6,3,4-Br(EtO)2C6H2CO2Me (VII), needles, m. 55-7°. p-KOC6H4Me (from 1.1 g. p-HOC6H4Me and 0.6 g. KOH), 2.6 g. IV, 0.1 g. Cu, and 0.1 g. (AcO)2Cu heated 4 hrs. at 190-200°, and the product extracted with Et2O and washed with 3% KOH gave 1.2 g. 4-[6,3,4-Me(EtO)2C6H2O]C6H4Me (VIII), b_p 130-57°. VIII (0.5 g.) and 35 ml. C5H5N-H2O treated with 5 g. KMnO4 portionwise, and the product concentrated extracted with Et2O, and dried in vacuo gave 4-[6,3,4-HO2C(EtO)2C6H2O]C6H4CO2H (IX), needles, m. 240-2° (from MeOH); di-Me ester (X), columns, m. 105-7°. p-KOC6H4CO2Me (from 5.5 g. p-HOC6H4CO2Me), 0.5 g. Cu, 0.5 g. (AcO)2Cu, and 10 g. VII heated 5 hrs. at 190-200° and the product treated as in VIII gave 3.4 g. X, m. 106-8°.

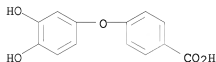
IT 859033-56-0P, Benzoic acid, p-(3,4-dihydroxyphenoxy)-

RL: PREP (Preparation)

(preparation of)

RN 859033-56-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L4 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:26059 CAPLUS

DOCUMENT NUMBER: 50:26059

ORIGINAL REFERENCE NO.: 50:5293f-i,5294d

TITLE: Dyes of the anthraquinone series. V.

3-Arylaminoalizarin

AUTHOR(S): Murata, Kazuya; Harada, Kozo; Takiyama, Ken

CORPORATE SOURCE: Hiroshima Univ.

SOURCE: Hiroshima Daigaku Kogakubu Kenkyu Hokoku (1955), 4, 387-90
 CODEN: HIDKAA; ISSN: 0018-2060

DOCUMENT TYPE: Journal

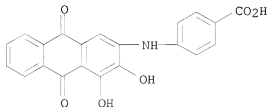
LANGUAGE: Unavailable

AB cf. C.A. 49, 2738d. To 0.5 g. 3-Aminoalizarin and 1 g. bromobenzene in 15 g. nitrobenzene, 0.2 g. AcONa and 0.07 g. CuCl₂ were added, and the reaction mixture was refluxed for 20 hrs., the solvent distilled off, and the residue was filtered, treated with dilute HCl, and then with dilute alkali to give 28% 3-anilinoalizarin, black-brown powder, m. above 300°, that vat-dyed rayon yellow-orange, and wool dark-purple-red with Cr as mordant, yellow-orange with Sn, and red-purple with Al. Similarly were prepared: 3-(4-nitroanilino)alizarin, m. above 300°, yield 22%, vat-dyed rayon in gray-yellow and wool brown-violet, yellow-orange, and gray-violet with Cr, Sn, and Al, resp.; 3-(2,4-dinitroanilino)alizarin, m. 296°, yield 68%, gave pale-brown rayon and orange-yellow, pale-orange-yellow, and pale-orange-yellow wool; 3-(4-carboxyanilino)alizarin, m. 287°, 29%, pale-brown and gray-violet, pale-orange-yellow, and pale-pink; 3-(p-sulfoanilino)alizarin, dyed wool black, yellow-orange, and black-purple; 3-(1-naphthylamino)alizarin, m. above 300°, 39%, pale-yellow-orange and pale-violet-brown, pale-yellow-orange, and dark-red; 3-(2-naphthylamino)alizarin, m. above 300°, 32%, pale-yellow-orange and pale-violet-brown, pale-yellow-orange, and pale-pink; 3-(1-anthraquinonylamino)alizarin, m. 294°, 73%, gray-brown and brown-violet, gray, and gray-purple; 3-(2-anthraquinonylamino)alizarin, m. above 300°, 30%, brown and brown, gray-orange, and brown; 3-(8-amino-1-anthraquinonylamino)alizarin, m. 298°, 67%, brown and pale-orange, -, and pale-brown; 3-(2-methyl-1-anthraquinonylamino)alizarin, m. above 300°, 22%, pale-pink and red-purple, pale-orange-brown, -; 1,8-bis(3-alizarylamino)anthraquinone, m. above 300°, 19%, brown and dark-red-purple, pale-orange, and pink; 1,5-bis(3-alizarylamino)anthraquinone, m. above 300°, 57%, brown and dark-purple, pale-orange, and pink; 2,6-bis(3-alizarylamino)anthraquinone, m. above 300°, 68%, gray-brown, and gray-brown-violet, pale-yellow-orange, and red-orange; 1,5-bis(3-alizarylamino)-4,8-dihydroxyanthraquinone, m. above 300°, 35%, gray-violet and gray-violet, gray-brown, and pale-brown; di-3-alizarylamine, m. above 300°, 35%, gray-brown and gray-black, pale-orange, and brown.

IT 859032-73-8P, Benzoic acid, p-(3,4-dihydroxy-2-anthraquinonylamino)-
 RL: PREP (Preparation)
 (preparation of)

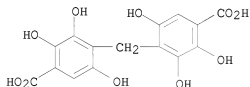
RN 859032-73-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L4 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1955:13586 CAPLUS
 DOCUMENT NUMBER: 49:13586
 ORIGINAL REFERENCE NO.: 49:2684c-f
 TITLE: Hyaluronidase-inhibiting substances
 INVENTOR(S): Hahn, Ladislaus; Fekete, Janos
 PATENT ASSIGNEE(S): Aktieselskabet "Ferrosan"
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	US 2688036		19540831	US 1952-308702	19520909 <--
AB	<p>Products obtained by condensation of 2,3,4-, 2,3,5-, 2,4,5-, and 2,4,6-trihydroxybenzoic acid with HCHO have a hyaluronidase-inhibiting power > 3000 times greater than salicylic acid and > 30 times greater than previously described inhibitors. Clinical tests indicate value in treatment of rheumatoid arthritis and certain infectious diseases. Thus, 2,4,6-trihydroxybenzoic acid (17 g.) was suspended in 100 g. cold 50% H₂SO₄ and 4 g. 40% HCHO was added. The reaction mixture was boiled for 5 hrs. with vigorous agitation. The warm product was filtered and the precipitate pulverized and washed with hot water. The product consisted essentially of polycondensed 2,2',-4,4',6,6'-hexahydroxy- 3,3'-dicarboxydiphenylmethane units. The relative hyaluronidase-inhibiting power was 3875 (salicylic acid = 1). Polycondensed products consisting of 2,2',3,3',4,4'-hexahydroxy-5,5'-dicarboxydiphenylmethane, 2,2',3,3',6,6'-hexahydroxy-4,4'-dicarboxydiphenylmethane, and 2,2',5,5',6,6'-hexahydroxy-3,3'-dicarboxydiphenylmethane units showed relative inhibitory powers of 3500, 4000, and 3100-50. Their preparation is described.</p>				
IT	857539-72-1, Benzoic acid, 4,4'-methylenebis[2,3,5-trihydroxy- (and polycondensed products)				
RN	857539-72-1 CAPLUS				
CN	Benzoic acid, 4,4'-methylenebis[2,3,5-trihydroxy- (CA INDEX NAME)				



L4 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1951:52800 CAPLUS
 DOCUMENT NUMBER: 45:52800
 ORIGINAL REFERENCE NO.: 45:8996h-i,8997a-e
 TITLE: The synthesis of certain substituted diaryl sulfones
 AUTHOR(S): Ettel, V.; Semonsky, M.; Cerny, A.
 CORPORATE SOURCE: United Chem. Met. Works, Prague-Vysocany

SOURCE: Collection of Czechoslovak Chemical Communications (1950), 15, 653-8
CODEN: CCCCAK; ISSN: 0010-0765

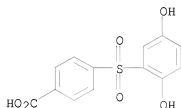
DOCUMENT TYPE: Journal

LANGUAGE: English

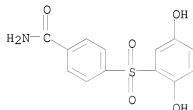
AB The sulfones reported below were without marked antibacterial activity, even against Mycobacterium tuberculosis. p-NCC6H4SO2H dissolved (5 g.) in 20 cc. boiling water was gently heated 10 min. with 32 g. p-quinone (I) in 10 cc. EtOH, the mixture filtered with charcoal, and the crystals which separated in the cold washed with water and recrystd. 3 times from water, yielding 2-(p-cyanophenylsulfonyl)hydroquinone (II), colorless needles, m. 182-3°. II (1.5 g.) dissolved in 10 cc. H2SO4 (d. 1.84), with cooling under water, was allowed to stand 5 days at room temperature in the open, then poured over ice, the resulting oil crystallized on standing and recrystd. from water gave 1.56 g. p-(2,5-dihydroxyphenylsulfonyl)benzamide (III), colorless rods, m. 236-7°. III (1.5 g.) refluxed 6 hrs. with 30 cc. of 40% H2SO4 and the product which separated on cooling filtered off, washed with water, and dried at 45°, yielded 1.5 g. p-(2,5-dihydroxyphenylsulfonyl)benzoic acid (IV), colorless, m. 295-6° (decomposition) (from MeOH). A solution of 5.4 g. II in 20 cc. absolute EtOH was saturated with HCl gas at 0°, allowed to stand 48 hrs., and the resulting Et p-(2,5-dihydroxyphenylsulfonyl)benzimidate-HCl (V) washed with 5 cc. EtOH, then 10 cc. dry Et2O, and kept over concentrated H2SO4; precipitation of the filtrate with Et2O gave addnl. V (total yield, 6.1 g.), colorless, m. 152-3°. V (2.5 g.) suspended in 10 cc. cold EtOH was allowed to stand 3.5 hrs. in 5 cc. of absolute alc. NH3 (7.5%) at room temperature, and the crude p-(2,5-dihydroxyphenylsulfonyl)benzimidine (VI) filtered off at the pump, washed with water, then EtOH, and dried in vacuo over KOH; addnl. VI, separated from the filtrate overnight. VI repeatedly crystallized from EtOH with alc. NH3, formed yellow microcrystals, m. 241-2°; picrate (prepared from V), m. 242-4° (decomposition) (from aqueous EtOH). p-NCC6H4SO2H (10 g.) dissolved in 45 cc. boiling water was gently heated 10 min. with 9.8 g. thymoquinone (VII) in 60 cc. EtOH, and filtered with charcoal; the oil which separated, crystallized in the cold, yielding 17 g. 3-(?)-(p-cyanophenylsulfonyl)thymohydroquinone (VIII), faintly yellowish, m. 152-3° (from aqueous EtOH). Crude 4,3-HO(HO2C)C6H3SO2Cl (from 56 g. of the SO3H acid) was shaken with 252 g. NaHSO3 in 500 cc. water (the solution being kept alkaline by slow addition of 50% NaOH during reaction), the cooled filtrate acidified with 60% H2SO4, and the 5-sulfinosalicylic acid (IX) filtered off and dried at 40°; yield, 35-7 g., m. 202-5° (decomposition, sealed tube). IX (10 g.) in 40 cc. of 10% H2SO4 stirred constantly at 70° with 4.8 g. I in 50 cc. water, and the solution cooled, gave white crystals of 2-(4-hydroxy-3-carboxyphenylsulfonyl)hydroquinone (X); repeated recrystn. from aqueous EtOH yielded X.H2O, m. 234-7° (decomposition). A IX (4 g.) in 30 cc. of 50% aqueous EtOH slowly added at 70° to 3 g. VII in 10 cc. of EtOH gave a brick-red oil; the cold solution was diluted with water, and the oil separated and kept in a desiccator over silica gel until it was triturated with CHCl3, giving 3-(?)-(4-hydroxy-3-carboxyphenylsulfonyl)thymohydroquinone (XI), colorless, m. 179-80° (from xylene). The solubilities of the above compds. are reported in general terms for various organic solvents.

IT 859033-53-7P, Benzoic acid, p-(2,5-dihydroxyphenylsulfonyl)-

860683-03-0P, Benzamide, p-(2,5-dihydroxyphenylsulfonyl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 859033-53-7 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED



RN 860683-03-0 CAPLUS
 CN Benzamide, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)



L4 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1951:41344 CAPLUS
 DOCUMENT NUMBER: 45:41344
 ORIGINAL REFERENCE NO.: 45:7048e-i,7049a-i
 TITLE: Aromatic keto- and hydroxy-polyethers as lignin models. III
 AUTHOR(S): Leopold, Bengt
 CORPORATE SOURCE: Kgl. Tek. Hogskolan, Stockholm
 SOURCE: Acta Chemica Scandinavica (1950), 4, 1523-37
 CODEN: ACHSE7; ISSN: 0904-213X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 45:41344
 GI For diagram(s), see printed CA Issue.
 AB cf. C.A. 44, 7338g. A series of lignin models of type (I) were synthesized and oxidized with PhNO₂ and alkali; oxidation was preceded by alkaline fission of the ether linkages. In all expts. 0.5-2 g. substance was heated 2 hrs. at 180° with 60 cc. of 2 N NaOH and 8 cc. PhNO₂/g. substance. The yields of vanillin (II), vanillic acid (III), 5-formylvanillin (IV), and 2,3,5-HO(MeO)(OHC)C₆H₂CO₂H (V) in Series A (I, R' = CH:CHMe), from (VI) (R = H, n = 0), (VII) (R = H, n = 1), (VIII) (R = Me, n = 0), and (IX) (R = Me, n = 1) were 69, 6, 1, and 11; 66, 8, trace, and 9; 0, 0, -, and -; and 70, 3, 2, and 12%, resp. The yield of II in Series B (I, R' = Pr) from (X) (R = H, n = 0), (XI) (R = H, n = 1), (XII)

(R = Me, n = 1), and (XIII) (R = Me, n = 2) was 60, 67, 67, and 62%, resp., and of III 6, -, 5, and -, resp. In series C, compds. of type 4,3-HO(MeO)C6H3R (XIV) were oxidized. The yield of II for R = CH2OH, CH2SO3(Ba/2), CH:CH2, Ac, COCH2OH, Pr, COEt, COCH(OH)Me, CH2CH:CH2, CH:CHMe, and CH:CHCHO in XIV was 82+, 80, 80, 81, 66, 17, 30, 33, 88, 90, and 86%, resp., and the yield of III was 3, -, 6, 4, 10, -, -, 21, -, trace, and 4%, resp. In Series D, compds. of type 5,4,3-R'(HO)(MeO)C5H2R (XV) were oxidized. The yields of II, IV, and V from (XVI) (XV, R = R' = CH2OH), (XVII) (R = CH2CH:CH2, R' = CH2OH), (XVIII) (R = CHO, R' = CH2CH:CH2), and IV (R = R' = CHO) were 0.8, 13, and 6; 2.2, 9, and 11; 1.6, 20, and 6; and 1.5, 12, and 26% resp. In series E, compds. of type (XIX) were oxidized. The yield of II from XIX (R = H, n = 2, 3, and 4) and XIX (R = Me, n = 2, 3, and 4) was 63, 60, 60, 88, 71, and 73% resp., and the yield of III was 11, 12, -, 0, 4, and -, resp. In Series F, compds. of type (XX) were oxidized. The yield of II from XX (X = OH, n = 2, 3, 4) and XX (X = SO3(Ba/2), n = 2, 3, and 4) was 87, 74, 72, 83, 70, and 71%, resp. Some members of series E (XIX, R = Me, n = 2 and 3) and Series F (XX, X = OH, n = 2 and 3) were heated 2 hrs. at 180° with 60 cc. 2 N NaOH to yield 14, 18, 3, and trace %, resp., of veratric acid and 75% acetoguaiacone (XXI), 75% XXI (and 12% III), 18% vinyl guaiacol (XXII), and 23% XXII, resp. In the preparation of dehydrodiisoeugenol (VI), to 50 g. freshly distilled isoeugenol in 450 cc. 95% EtOH and 200 cc. H2O, were added 70 g. FeCl3 in 200 cc. H2O and a few crystals VI, the mixture cooled, and the precipitate of VI separated, washed with 45% EtOH, and recrystd. from

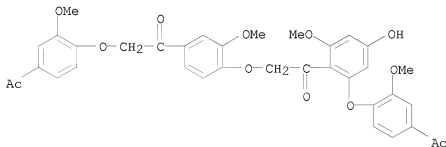
EtOH;

the yield of VI was 15 g., m. 132-3°. In the preparation of (acetoguaiacyl)dehydrodiisoeugenol Me ether (IX), 5 g. α-bromoacetoveratrone (XXIII), 6.3 g. VI, and 10 g. anhydrous K2CO3 in 100 cc. absolute MeCOEt were refluxed 30 min., the mixture washed with H2O, and the MeCOEt layer dried over anhydrous Na2SO4 and concentrated in vacuo to yield 7.95 g. IX, m. 123-4° (from EtOH). (Acetoguaiacyl)dehydrodiisoeugenol benzoate (XXIV) was prepared by treating 4.2 g. 3,4-MeO(BzO)C6H3COCH2Br (XXV), 4 g. VI, and 10 g. K2CO3 in 100 cc. MeCOEt as above; the yield of XXIV was 3.7 g., m. 124-5° (from EtOH). XXIV (2.7 g.) refluxed with 2 cc. piperidine (XXVI) in 75 cc. EtOH 30 min., and the mixture poured into H2O, acidified, and treated with EtOH, yielded 1.6 g. crystals which were dissolved in CHCl3, the solution filtered through Al2O3, and the CHCl3 evaporated to yield (acetoguaiacyl)dehydrodiisoeugenol (VII), m. 129-30° (from dilute EtOH). Acetoguaiacyldihydrodehydrodiisoeugenol Me ether (XII), m. 99-100°, was prepared in 78% yield from XXIII and X as described above for IX; di(acetoguaiacyl)dihydrodehydrodiisoeugenol Me ether (XIII) (I, R' = Pr, R = Me, n = 2), m. 114-15°, in 79% yield from o-bromoacetoguaiacylacetoguaiacone Me ether and X. XI benzoate, m. 98-9°, in 54% yield from XXV and X, and XI, m. 82-3°, in 73% yield by the debenzoylation of XI benzoate with XXVI. Methylation of XI with CH2N2 in Et2O gave XII, m. 100-101°. Dihydro-3-methoxy-4-benzoyloxyphenacyl coerlignol ether (XXVII) was prepared as follows: To 10 g. XXI and 15 cc. PhCH2Cl in 150 cc. EtOH was added 3.7 g. NaOH, the mixture refluxed 1.5 hrs., poured into H2O, extracted with Et2O, and the Et2O solution washed with H2O, dried over anhydrous Na2SO4, and evaporated to yield an oil from which was separated 13.3 g. acetoguaiacone benzyl ether, 4,2-Ac(MeO)C6H3OCH2Ph (XXVIII), m. 86-6.5° (from petr. ether). To 10 g. XXVIII in 100 cc. CHCl3 was added 6.25 g. Br in 50 cc. CHCl3, and the mixture washed with NaHCO3 solution and H2O, dried over anhydrous Na2SO4

and

evaporated to yield 9.7 g. *m*-bromoacetoguaiacone benzyl ether (XXIX), m. 102.5-103° (from C6H6-petr. ether). XXIX (5 g.) and 2.55 g. coerulignol, treated as described for the preparation of IX, yielded 5.5 g. 3-methoxy-4-(benzyloxy)phenacyl coerulignol ether, m. 86.5-7.5° (from Et2O), 4 g. of which with 4 g. (Me2CHO)3Al in 30 cc. absolute iso-PrOH yielded 3.5 g. XXVII, m. 55-7°, which in vacuo at 70° lost 1 mole H2O to give anhydrous XXVII, m. 62-3°. The oxidation products were steam-distilled to remove nitrogenous compds., acidified, extracted continuously for 24 hrs. with C6H6, and the C6H6 exts. shaken with bisulfite, bicarbonate, and NaOH. A detailed description is given for the separation and identification of the oxidation reaction products. In general it was found that units connected only by ether linkages gave high yields of II and III, and units connected by C-C linkages gave no II or III.

IT 857560-43-1P, Acetophenone, 2'-[2-(4-acetyl-2-methoxyphenoxy)-4'-(4-hydroxy-2-methoxyphenacyloxy)-2,4'''-oxybis[3'-methoxy-
RL: PREP (Preparation)
(preparation of)
RN 857560-43-1 CAPLUS
CN Ethanone, 2-[4-[2-(4-acetyl-2-methoxyphenoxy)acetyl]-2-methoxyphenoxy]-1-[2-(4-acetyl-2-methoxyphenoxy)-4-hydroxy-6-methoxyphenyl]- (CA INDEX NAME)



L4 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1949:41364 CAPLUS

DOCUMENT NUMBER: 43:41364

ORIGINAL REFERENCE NO.: 43:7449g-i,7450a-f

TITLE: Compounds related to 4,4'-diaminodiphenyl sulfone.
p-Arylsulfonylphenylethylamines and related compounds

AUTHOR(S): Burton, H.; Hu, P. F.

SOURCE: Journal of the Chemical Society (1949)
178-81

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

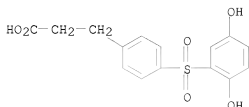
AB cf. C.A. 42, 6356ag. 4-O2NC6H4SO2C6H4Me-4 with CrO3 in AcOH-Ac2O-H2SO4 gives 4-(p-nitrophenylsulfonyl)benzylidene diacetate, m. 150-1°; hydrolysis gives 74% 4-(p-nitrophenylsulfonyl)benzaldehyde, m. 214-15°. 2,5-(HO)2C6H3SO2C6H4CN-4 with the Stephen reagent from 9 g. anhydrous SnCl2 in 130 cc. ether (shaken 7 hrs.) gives 5 g. 4-(2,5-dihydroxyphenylsulfonyl)benzaldehyde, m. 200-1°. p-MeO3C6H4CHO (6 g.), 7 g. hippuric acid, 8 g. AcONa, and 30 cc. Ac2O, heated 1 hr. on the steam bath, give 5 g. 5-keto-2-phenyl-4-(p-

methylsulfonylbenzylidene)-4,5-dihydrooxazole (I), yellow, m. 186-7°; hydrolysis of I with warm dilute NaOH gives α -benzamido-p-(methylsulfonyl)-cinnamic acid (II), m. 245-6° (decomposition). Analogs of I: 4-(p-Phenylsulfonyl), yellow, m. 222-3°, 73%; 4-(4-p-chlorophenylsulfonyl), orange-red, m. 212-13°, 60%; 4-(4-p-methoxyphenylsulfonyl), yellow, m. 195-6°, 90%; 4-(p-N-acetylsulfonyl) analog (III), orange-red, m. 240-1° (decomposition), 62%. p-PhSO₂ analog of II, m. 226-7°. I (9 g.), reduced with 5.6 g. red P and 35 cc. HI in 35 cc. Ac₂O, gives 5.5 g. (p-RSO₂C₆H₄)CH₂CH (NH₂) CO₂H, where R is Me, m. 270° (decomposition). The following were similarly prepared (R given): Ph, m. 252° (decomposition), 70%; p-chlorophenyl, m. 259° (decomposition), 73%; p-hydroxyphenyl, with 1 mol. H₂O, m. 265° (decomposition), 62% from the MeO compound; p-aminophenyl (IIIA), yellow, m. 195° (decomposition), 40%. III (5 g.) in 60 cc. EtOH at 75°, treated with 26 g. 3% Na-Hg and, after 1.5 hrs., with an addnl. 26 g., with stirring for an addnl. 2.5 hrs., and the residue in 15 cc. H₂O acidified with concentrated HCl, gives α -benzamido- β -(p-sulfamylphenyl)alanine-HCl, m. 237° (decomposition). The acids could not be decarboxylated by heating alone in vacuo or in C₃H₅(OH)₃, Ph₂NH, or paraffin. The appropriate aldehyde, heated at 100° with CH₂(CO₂H)₂ in C₅H₅N containing a little piperidine until effervescence ceases and then treated with an excess 6 N HCl, gives 67-87% of the p-(R-sulfonyl)cinnamic acids, p-RSO₂C₆H₄CH:CHCO₂H (R given): Ph, m. 298°; p-chlorophenyl, m. 282°; p-methoxyphenyl, m. 259-61° (decomposition); p-nitrophenyl (IV), m. 273-5°; amino (V), m. 276° (decomposition). The Na salts in H₂O were reduced over Raney Ni at room temperature and atmospheric pressure, giving 77-90% of the β -[p-(R-sulfonyl)phenyl] propionic acids: R = Ph, m. 194-5°; p-methoxyphenyl, m. 168°; 2,5-dihydroxyphenyl, m. 180°. Catalytic reduction of IV gives the p-aminophenyl analog [HCl salt, m. 209° (decomposition); Ac derivative, with 1 mol. H₂O, m. 215°]. Reduction of IV with Fe powder in aqueous EtOH containing HCl gives p-(4-aminophenylsulfonyl)cinnamic acid, whose Ac derivative m. 237°. Reduction of 3 g. V with 3% Na-Hg in dilute NaOH gives 2.5 g. β -(p-sulfamylphenyl)propionic acid (VI), m. 148-50°. The 2-[p-(R-sulfonyl)phenyl]ethylamine-HCl were prepared in 40-60% yields from the propionic acids through the acid chlorides and azides (R given): Ph, m. 184-5°; p-chlorophenyl, m. 251°; p-methoxyphenyl, m. 170°; 2,5-dihydroxyphenyl, m. 197°; p-aminophenyl (free base), m. 129°; amino (VII), m. 149°. 1-[p-(R-sulfonyl)phenyl]ethylamines were prepared in 50-66% yields from the reaction of the appropriate ketone and 4 mols. HCO₂NH₄ and hydrolysis of the insol. material with boiling concentrated HCl: Ph, m., 85° (HCl salt, m. 218-19°); amino, m. 172°. p-Methylsulfonyldiphenylamine, Ph(MeSO₂C₆H₄)CHNH₂ (VIII), m. 92-3°; p-PhSO₂ analog, m. 154-5°, 80%. p-H₂NC₆H₄Ac gives 20% 4,4'-diacetyldiphenyl disulfide, m. 92-3°; 2.4 g. yields 1 g. p-sulfamylacetophenone, m. 178-9°. p-AcC₆H₄N₂Cl and Na₂S give 4,4'-diacetyldiphenyl sulfide, m. 88°, which yields 4,4'-diacetyldiphenyl sulfone, m. 209°. VI-VIII had little or no activity against *Streptococcus hemolyticus* at a dilution of 1:1000. IIIa is also inactive.

IT 858215-86-8P, Hydrocinnamic acid, p-(2,5-dihydroxyphenylsulfonyl)-860679-98-7P, Benzaldehyde, p-(2,5-dihydroxyphenylsulfonyl)-
 RL: PREP (Preparation)
 (preparation of)

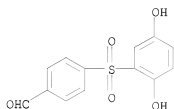
RN 858215-86-8 CAPLUS

CN Benzenepropanoic acid, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)



RN 860679-98-7 CAPLUS

CN Benzaldehyde, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)



L4 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1928:13476 CAPLUS

DOCUMENT NUMBER: 22:13476

ORIGINAL REFERENCE NO.: 22:1583h-i,1584a-e

TITLE: Reactions of diazomethane on ethyl
phloroglucinoldicarboxylate and its derivatives and
their reaction with nitric acid

Leuchs, Hermann

SOURCE: Justus Liebigs Annalen der Chemie (1928),
460, 1-32

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB (With Ilse Waldorf). The ester, C₁₂H₁₄O₇ (3.87 g.), 0.25 g. FeCl₃ and 3 g. BzCl in 50 cc. ligroin, boiled 1 hr., give 0.6-1.2 g. Et O-benzoylphloroglucinoldicarboxylate (I), m. 137-8°; FeCl₃ gives a red color; an oxime could not be prepared; with AcCl it gives the tri-Ac derivative, m. 96-8°. I (1.25 g.) and 0.5 g. CH₂N₂ in Et₂O, allowed to stand 1 hr. between 0° and 20°, give 0.4-0.6 g. of the O-di-Me ether (II) m. 106°, and 0.8-0.6 g. of the O-mono-Me ether, m. 116-8°. II is saponified by EtOH-NaOH, giving Et O-dimethylphloroglucinoldicarboxylate (III) m. 146-7°; the free acid, m. 186-8° (decomposition); BrHBr in AcOH gives the compound C₉H₉O₅Br, m. 220° (decomposition). III is also obtained by the methylation of the ester at 15° (2.2 mols. CH₂N₂; 1.2 mols. CH₂N₂ give 40% of the mono-Me ether, m. 107.5-8.5°. O-Trimethylphloroglucinoldicarboxylic acid (IV), decomp. 260°, is

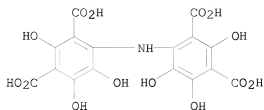
obtained by saponification of the ester by EtOH-NaOH; with Br it gives dibromophloroglucinol tri-Me ether, m. 129-30°. The Br derivative of IV, m. 165-73° (decomposition) is obtained by saponification of the ester, m. 51°. The Nitro derivative of IV, m. 132-5°, decomps. 180°, is likewise obtained by saponification of the ester, b15 about 250°; with CH2N2 the acid gives the di-Me ether, m. 70-1°.

Nitrophloroglucinol tri-Me ether, m. 151-2°. Et 1,2,3,5-tetramethoxybenzenedicarboxylate, from the phenol and CH2N2, m. 64-5°. Et N-dimethylaminophloroglucinoldicarboxylic acid, m. 151-2°; FeCl3 gives a red color. Et O-trimethylphloracetophenenedicarboxylate, from the phenol ester and CH2N2, oily; the free acid, m. 142-4°, decomps. 170°; CH2N2 and the acid give the di-Me ester, m. 74°. (With Paul Sander.) The action of HNO3 (d. 1.39) on the ester C12H14O7 at 10-25° gives 46-56% of tetra-Et phlorazurintetracarboxylate (V), C24H23O14N (formerly considered a ketenequinone, C22H21O13N, C. A. 3, 542), m. 162-3°; CH2N2 gives a dark red tri-Me ether, m. 100-1°; heating V in AcOEt or C6H6 gives 55-62% of the compound C22H19O13N (VI), light reddish brown, m. 230-2°. V and CH2N2 give the dark red compound, C26H27O13N, m. 109-10°, reduced by Zn dust in AcOH to the yellow compound, C24H29O13N, m. 136°. Reduction of VI with Zn and AcOH gives the compound C22H21O13N, yellow, m. 198-212°; CH2N2 gives the compound, C27H31O13N, m. 120-1°. (With W. Robert Leuchs.) Reduction of VI gives tetra-Et trihydroxyphenoxazine-1,3,6,8-tetracarboxylate, brick-red, m. 192-3°, whose tri-Ac derivative m. 172-4°. CH2N2 gives the O-tri-Me derivative, light yellow-red, m. 112-3°, reduced by Zn in AcOH to the tri-Me derivative of the oxazine, C27H31O13N, pale yellow, m. 119.5-20.5°. EtOH-NH2OH gives a red oxime, C12H14O7N2 (VII), m. 138°, and a yellow oxime, C12H13O13N (VIII), m. 141°. HNO3 oxidizes VII to Et nitrophloroglucinoldicarboxylate. Reduction of VII with Zn in AcOH gives the diamine, C12H16O6N2, m. 126-7°; CH2N2 gives the compound C13 H14O6N2, m. 130-2°. VIII gives the same oxidation product as VII; CH2N2 gives the compound C14H15O7N, m. 162-3°. Tetra-Et tetrahydroxyphenoxazine-1,3,6,8-tetracarboxylate, golden yellow, m. 195-7°; it crystals with 14% AcOH, m. 185-7°; O-tetra-Me derivative, light yellow, m. 98-9°. The yellow acid, C24H23O14N (C. A. 3, 542) (IX) is obtained from the ester C12H14O7 with HNO3 (d. 1.45) in 40-50% yields, together with 30-40% of the nitro ester, C12H13O8N; IX decomps. at 216°; the di-Ac derivative, m. 185-7° (Me ester, m. 140-2°). IX yields a tri-Me derivative, m. 96-8°. Reduction of IX gives the compound C24H25O14N, m. 145-7°. IX and NH2OH in EtOH-KOH give the compound C21H21O12N3, sinters 187°, decomps. 207° (HNO3 gives the compound C21H20O12N2, m. 153-4°), and the monoxime, C23H24O12N2, m. 130-1° (di-Me ether, m. 67-8°). Tetra-Et sym-hexahydroxydiphenylaminetetracarboxylate, C24H27O14N, m. 186-7°; Ac derivative, m. 207-8°; a by-product is the greenish yellow compound C24H25O13N, m. 187° (tetra-Ac derivative, m. 204-5°; di-Me ether, yellow, m. 124-5°; tri-Me ether, yellow, m. 84-6°).

IT 857806-18-9, Isophthalic acid, 4,4'-iminobis[2,5,6-trihydroxy- (derivs.)

RN 857806-18-9 CAPLUS

CN Isophthalic acid, 4,4'-iminobis[2,5,6-trihydroxy- (3CI) (CA INDEX NAME)



L4 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1909:250 CAPLUS

DOCUMENT NUMBER: 3:250

ORIGINAL REFERENCE NO.: 3:55i,56a-h

TITLE: Carbomethoxy Derivatives of Phenolcarboxylic Acids and

their Employment for Syntheses

AUTHOR(S): Fischer, Emil

CORPORATE SOURCE: Chem. Inst., Univ. Berlin

SOURCE: Berichte der Deutschen Chemischen Gesellschaft (

1909), 41, 2875-91

CODEN: BDCGAS; ISSN: 0365-9496

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB p-Carbomethoxyhydroxybenzoic acid, MeO2COC6H4CO2H, from p-hydroxybenzoic acid and methyl chlorcarbonate, in presence of 1N aqueous NaOH (cf. preceding abstract). Slender, colorless needles, m. 179° (corrected) previously softening. Yield quantitative. It gives no color with FeCl3 or Millon's reagent and is hydrolyzed immediately to the hydroxybenzoic acid by solution in cold aqueous NaOH. Chloride, from the acid and PCl5; long, colorless, radial needles, m. 82-3° (corrected) previously softening. It boils without decomposition (10-15 min.) and is relatively stable in air. Yield, 90%. Ethyl glycolate converts it into ethyl p-carbomethoxyhydroxy-benzoylglycinate, MeO2COC6H4CONHCH2CO2Et; colorless, lustrous plates, m. 63°, previously softening. Yield, practically quantitative. With alkali it gives p-hydroxyhippuric acid, HOC6H4CONHCH2CO2H, m. and decomposes 238° (240° corrected). Schotten gives m. 228°; his material was from the urine of dogs fed on p-hydroxy-benzoic acid and from that of men fed on Na hydro-p-cumarate. The acid may also be obtained from the chloride and glyccoll, in alkaline solution, but the yield is only 50 instead of 93%. The compounds described below were prepared in a similar manner to the preceding ones. Dicarbomethoxyprotocatechuic acid, (MeO2CO)2C6H3CO2H; colorless, slender needles, m. 165-6° (corrected), previously softening. Yield, 90%. Chloride, colorless needles, softens about 116°, m. 118° (corrected). Yield, 90-5%. Tri-carbomethoxygallic acid, (MeO2CO)3C6H2CO2H, was prepared in an atmosphere of H. Bundles of colorless, thin prisms, softens about 130°, m. 136-41° (corrected). Yield, 80-5%. Brom derivative, crystalline. Pyridine salt. In presence of excess of the base, the acid is hydrolyzed. Tricarbethoxygallic acid, colorless, lustrous plates, m. 96-7° (corrected), previously softening. Yield, almost quantitative. The carbomethoxy acid is hydrolyzed completely by heating with cold HCl (20%), or by the action of cold aqueous NaOH or NH3; with 2NaOH, at 20°, dicarbomethoxygallic acid is formed, colorless crystals resembling biconvex lenses, m. 160° (corrected), previously softening. Yield, 90%. It is probable that the OH is in the p-position.

Tricarbomethoxygalloyl chloride, long needles, m. 86° (corrected), previously softening. Yield, 94%. It gives colorless compounds with NH_3 and PhNMe_2 . Anilide, $(\text{MeO}_2\text{CO})_3\text{C}_6\text{H}_2\text{CONHPh}$ bundles of pointed needles, m. $175-6^{\circ}$, previously softening. Tricarbomethoxygalloyl-p-hydroxybenzoic acid, $(\text{MeO}_2\text{CO})_3\text{C}_6\text{H}_2\text{COOC}_6\text{H}_4\text{CO}_2\text{H}$, from the chloride, p-hydroxybenzoic acid and aqueous NaOH . Bundles of thin prisms, m. 165° (corrected), previously softening. Aqueous NH_3 hydrolyzes it to galloyl-p-hydroxybenzoic acid, $(\text{HO})_3\text{C}_6\text{H}_2\text{COOC}_6\text{H}_4\text{CO}_2\text{H}$ heavy, sandy lustrous, crystalline powder consisting of microscopic, acute angled plates, m., blackens and evolves gas about 260° (corrected). Yield, 60%. Its alkali solution quickly becomes brown in air and its color reactions with FeCl_3 and KNC resemble those of gallic acid. Alkalies hydrolyze it to its constituent acids. Tricarbomethoxy-galloyl chloride and dicarbomethoxygallic acid, in presence of NaOH , yield an amorphous compound, which, by the action of aqueous NH_3 , forms what is probably di-gallic acid. Thin, short, microscopic prisms, or needles, m., darkens and evolves gas about $275-80^{\circ}$. The applications of this method of synthesis are very numerous. Hitherto it had not been possible to prepare chlorides of phenolcarboxylic acids, because the PCl_5 attacked both the CO_2H and OH . The interaction of salicylic acid and methyl chlorcarbonate is attended with considerable difficulties, but methyl salicylate combines easily.

IT 861603-50-1P, Benzoic acid, p-(gallyl)-

RL: PREP (Preparation)

(preparation of)

RN 861603-50-1 CAPLUS

CN Benzoic acid, 4-[(3,4,5-trihydroxyphenyl)methyl]- (CA INDEX NAME)

